Dimethyl sulfoxide
67-68-5 | DTXSID2021735

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 11.2 days

Global applicability domain: Inside

Local applicability domain index: 4.36e-01

Confidence level: 7.10e-01

Nearest Neighbors from the Training Set

Image not found
1,2,4,5-Tetramethylbenzene
Measured: 88.3
Predicted: 5.46

Image not found
2,2-Dimethylbutane
Measured: 880
Predicted: 16.2

Image not found
2,2,3-Trimethylbutane
Measured: 61.9
Predicted: 10.7

Image not found
2,3,4-Trimethylpentane
Measured: 511
Predicted: 13.9

Image not found
Ethylcyclopentane
Measured: 511
Predicted: 8.14